Our choice of title may seem strange but we mean each word. In this talk, we are not going to be concerned with computations made “after the fact”, i.e. those for which data are available and which are being conducted for explanation and insight.

Here we are interested in preventing S&C design problems by finding them through computation before data are available. For such a computation to have any credibility with those who absorb the risk, it is necessary to quantitatively PREDICT the quality of the computational results.

Quantitative Prediction of Computational Quality

(so the S&C folks will accept it)

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NASA Symposium on Computational Methods for Stability and Control
September 23-25, 2003
Hampton, Virginia

Please note two things:

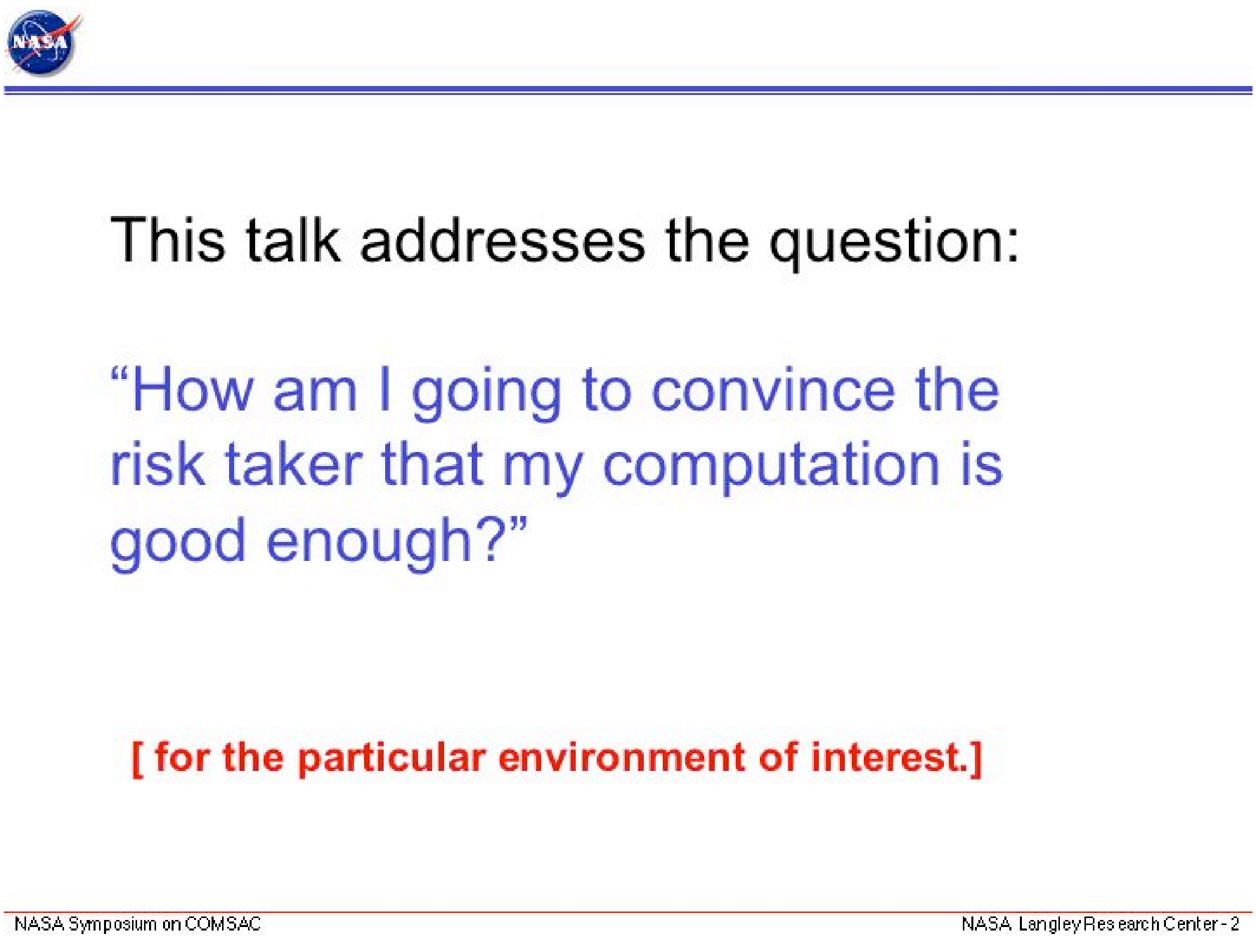
There are a large number of people at Langley Research Center who are working on these issues, but we got tasked with presenting this talk.

We do not claim that these notions are original to us, but the application and emphasis may be.

We want to make two points here:

1. No answer or a qualitative answer to the question “How good is my answer?” is not good enough for assessing risk. We will address this point in more detail later

2. Where insightful and accurate S&C predictions are most desperately needed is in the design environment. Making a computation after data have been obtained is not a prediction --- it is an explanatory effort. Explanatory efforts can be very useful but they do not require prediction of uncertainty. Note that attempts at calibration do, however, require uncertainty assessments of both the prediction and the experimental data. Otherwise, one has no idea how “fuzzy” the calibration/validation is.



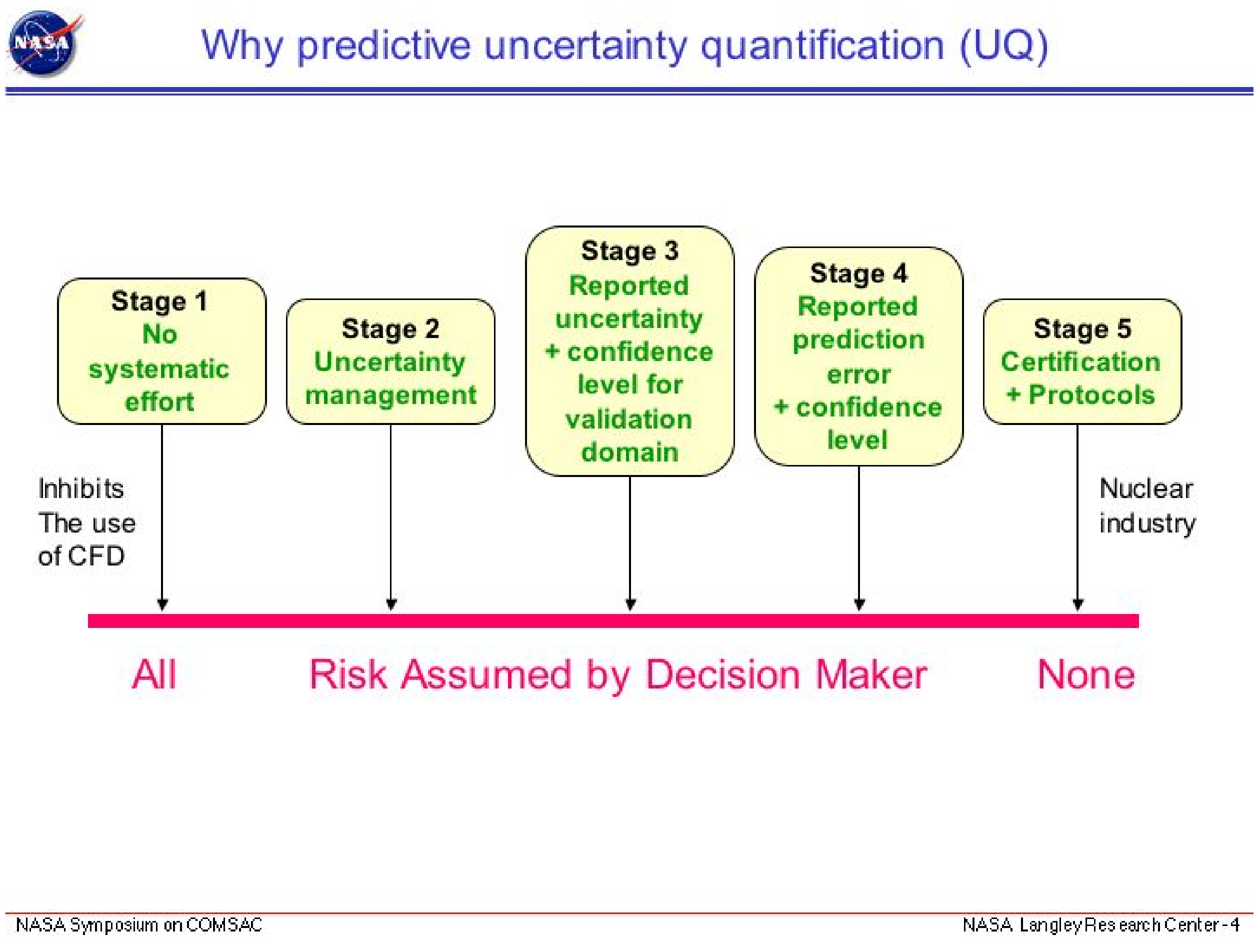
Outline

- Risk relates directly to the ability to quantitatively predict uncertainty
- An S&C example and its interpretation based on point-of-view
- Expanding the traditional quality question
- A long-term strategy for creating a controllable process
- A strategy for getting started
  - For getting useful results right now
  - For establishing the long-term process

This chart is designed to illustrate the relationship of uncertainty quantification to risk.

At the left end of the chart, there is no defined and managed process in place and no uncertainty quantification is possible. For this state of affairs, the decision maker, i.e. the person or group that uses the computational results, necessarily assumes all of the risk associated with any inaccuracy of the prediction.

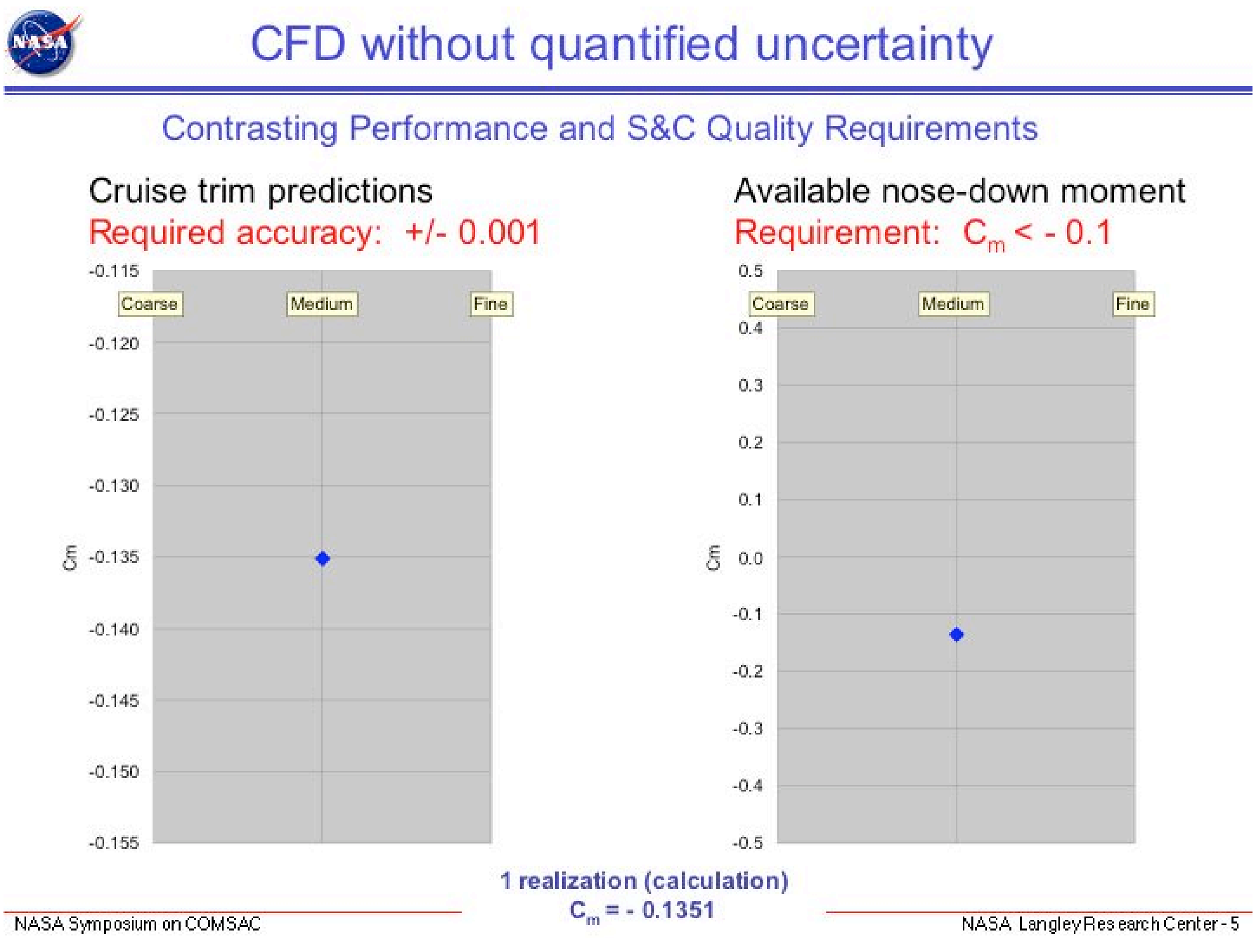
At the other end of the chart, the computationalist predicts the uncertainty following protocols and certification procedures suitable for use in a Court of Law. For this state of affairs, the risk is assumed entirely by the computationalist and he or she can be sued.



The other stages progress from the left to right, but please note that even the very first stage beyond the state of no quantification requires definition of a process and some sort of management system for verifying that the process is being followed.

Most (or virtually all) CFD is performed today without quantifying the consequences of uncertainty to an outcome metric. When uncertainty has been considered, it is usually restricted to a limited assessment of grid effects; other sources (turbulence model, algorithm, parameters, user practices, …) are generally left unaddressed.

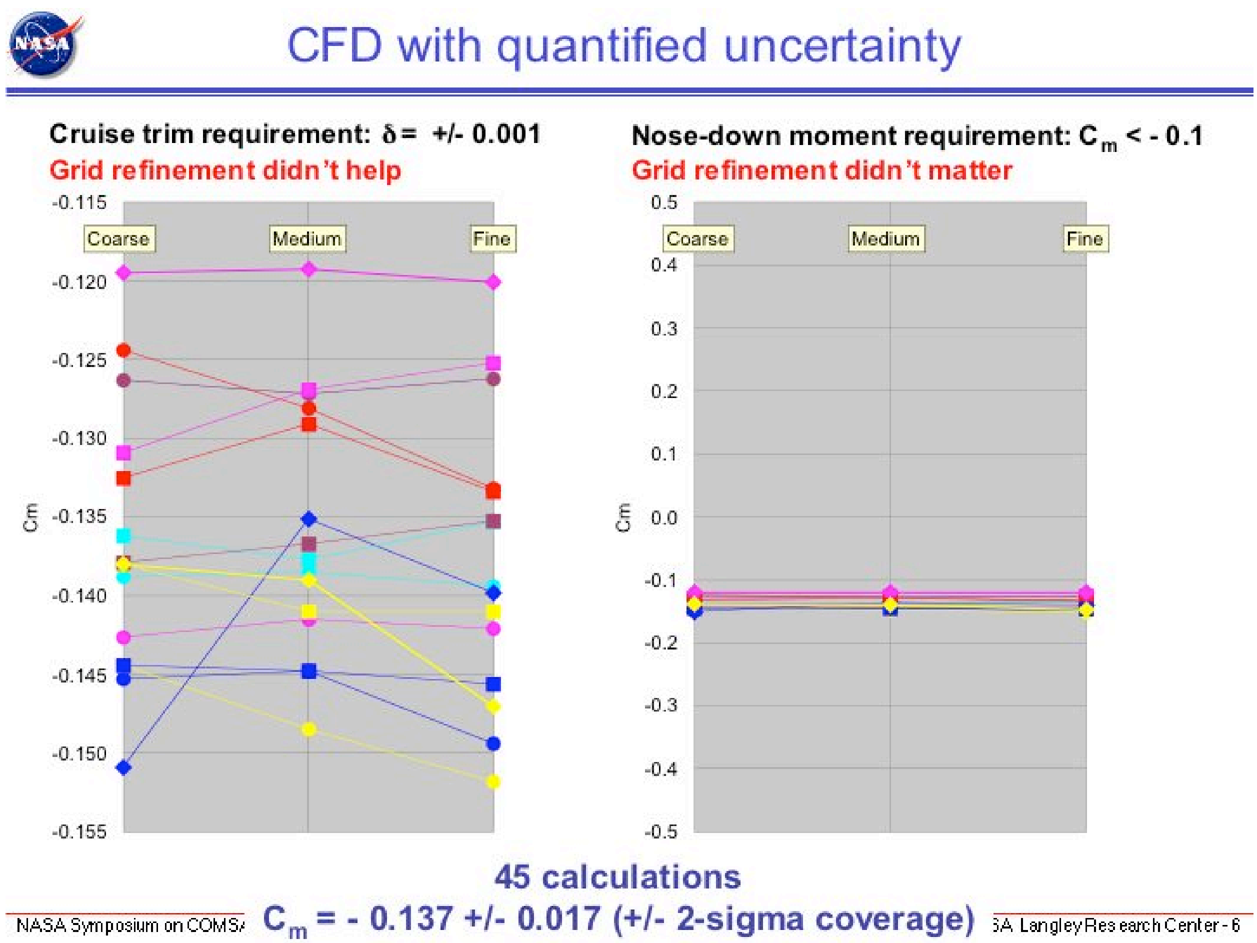
The chart contrasts two customer requirements for a CFD computation of pitching moment. On the left is a cruise transport trim application where the required accuracy of the Cm prediction is +/- 0.001. On the right is a high angle of attack S&C application where the performance requirement is to have at least -0.1 nose down authority. The scales are set accordingly for each customer requirement, and the chart also provides for some grid sensitivity information to be added.



In the absence of quantified uncertainty, all that known is the deterministic result that Cm = -0.1351. It is not know to any level of confidence if this calculation meets either customer's requirement. Under such circumstances, the prediction is of limited use.

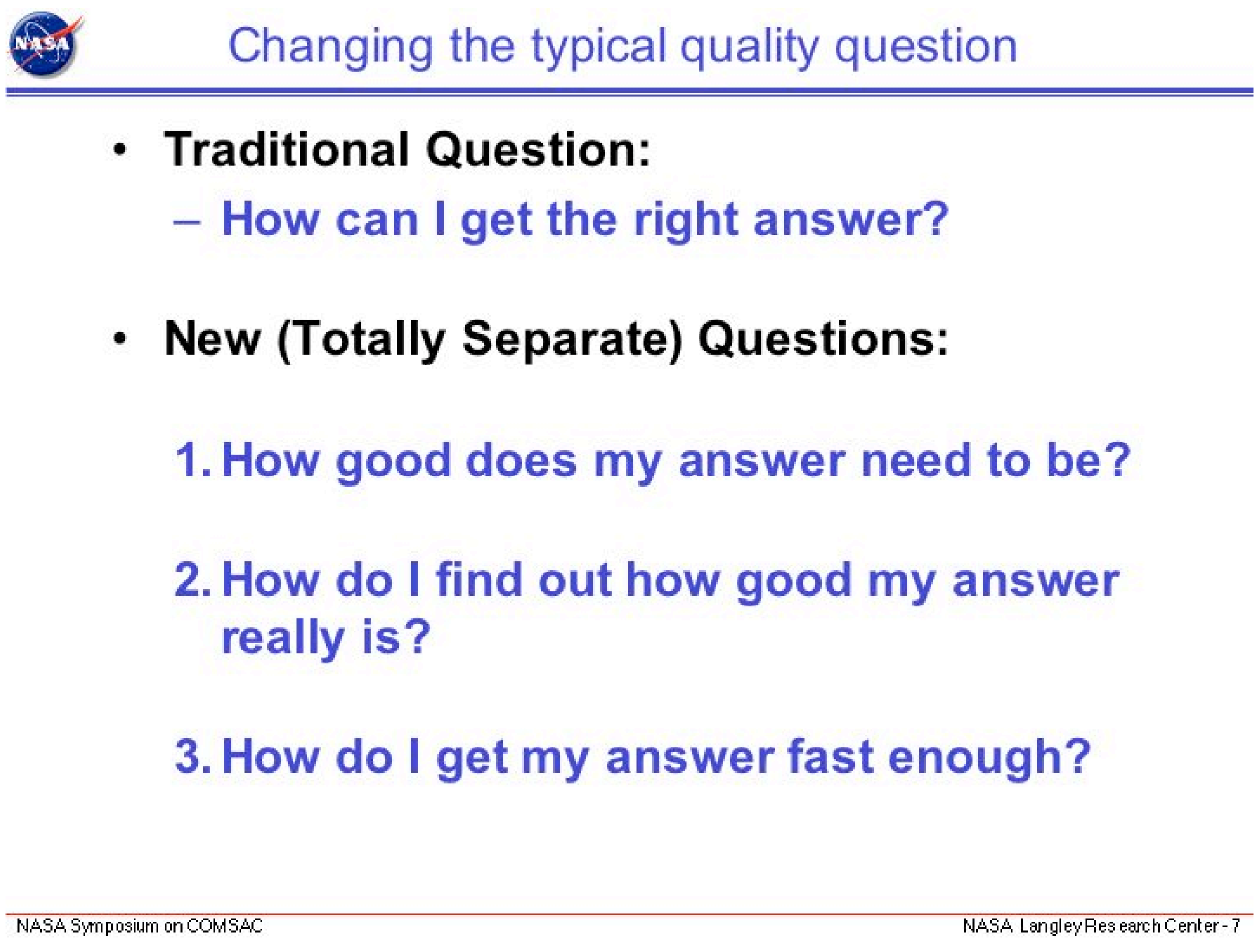
This figure has the identical format to the previous one. However, the results from a fairly extensive uncertainty quantification process are included. Forty-five computations were performed at three different grid density levels. Simple statistics now tell us that Cm = -0.137 +/- 0.017 at 95% confidence. This outcome includes a variety of uncertainty sources (different grids, different turbulence models, different flow solvers, etc.)

The individual results are also shown on both the left and right sides of the figure to put them in the context of the two customer requirements. It is clear that the variation is (1) completely unacceptable to the cruise trim requirement on the left and (2) completely acceptable to the high-a S&C objective on the right.



Simply put, uncertainty quantification entails determination of conventional terms (average, standard deviation, and confidence) subject to certain process requirements. However, practical techniques will be required to quantify computational uncertainty within available resources and on a timescale consistent to project requirements.

Looking at individual pieces of the quality problem shines more light on them and actually recognizes that they each require different processes and ways of thinking. They end up being separate disciplines which develop on their own and co-evolve as well.



The question “How good does my answer have to be?” can only be answered by the customer of the computational results, i.e. the risk taker. Of course, the customer should always be informed of the likely quality of the process before he/she commissions the work. Furthermore, the resources provided by the customer can have a significant impact on the possible quality of the computational results.

Unfortunately, the general absence of quantitative predictions of computational uncertainty has led to a typical customer demand of “Do the best you can.” However, recent efforts at several institutions to establish wind tunnel data quality assurance programs have encouraged some customers, most notably performance groups, to revisit their quality needs and to develop well-

Question 1

- **How good does my answer need to be?**
  (i.e. “What quantitative quality level is needed?”)
  - The customers, i.e. the user, of the computational predictions are responsible for determining their quantitative quality requirements.
  - Ideally, they would develop a process for doing this on a consistent basis.
  - This has nothing to do with the computational process and is not the subject of this talk.

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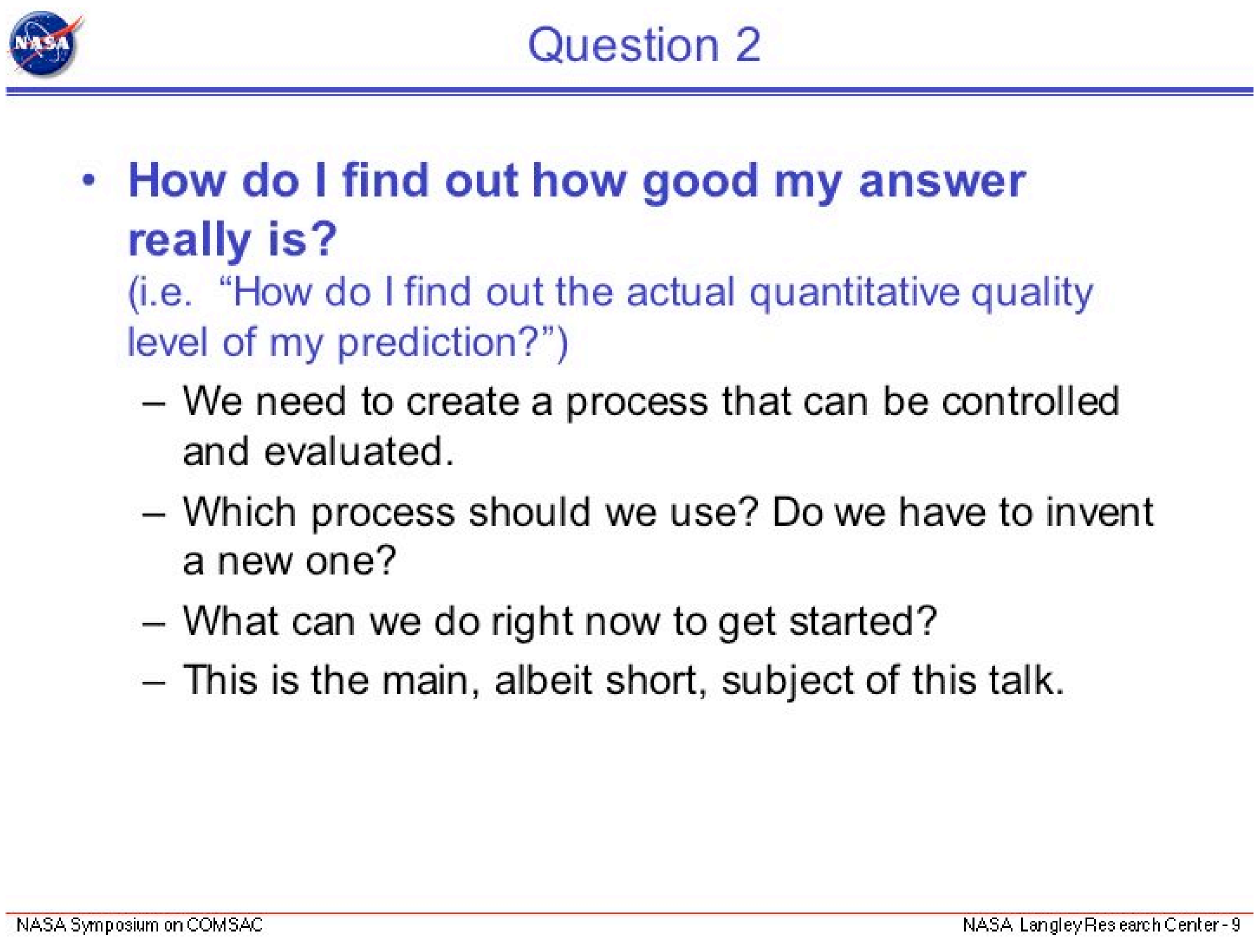
defined processes for establishing defendable uncertainty requirements. These uncertainty requirements are usually traceable to some design or regulatory requirement that must be met for the airframe program to succeed. Some of these requirements are not even technical in nature, but nevertheless must be met.

Answering this question is the present focus of the computational uncertainty quantification work at Langley Research Center. It is impossible in this short talk to address anything more than the general notions. We recommend the following references:

P. J. Roache, "Verification and Validation in Computational Science and Engineering", Hermosa, 1998.

W. L. Oberkampf, T. G. Trucano, "Verification and Validation in Computational Fluid Dynamics", Progress in Aerospace Sciences, Vol. 38, No. 3, 2002, pp. 209-272.

J. M. Luckring, M. J. Hemsch, J. H. Morrison, "Uncertainty in Computational Aerodynamics", AIAA-2003-0409, January 2003.



M. R. Mendenhall, R. Childs, "Best Practices for Reduction of Uncertainty in CFD Results", AIAA-2003-0411, January 2003.

M. J. Hemsch, "Statistical Analysis of CFD Solutions from the Drag Prediction Workshop", AIAA-2002-0842.

M. J. Hemsch, "Statistical Analysis of CFD Solutions from 2nd Drag Prediction Workshop", AIAA-2004-0556, January 2004.

This question really addresses the issue of what process do I need?

It is possible to use lower-order-physics codes for S&C problems as long as the domain of uncertainty predictability is known in advance. This means that the problem of interest would have to be pretty close to a previously-quantified domain.

For true prediction, when such a previously-quantified domain does not exist, quantified uncertainty prediction does not seem possible.

Note that this notion is especially important when novel configurations are being considered.

Question 3

- **How do I get my answer fast enough?**
  (i.e. "How do I get my predictive answer and its uncertainty fast enough?")
  - This is not the subject of this talk, but we can't resist a few comments.
  - Gotta have sufficient physics (or somehow put limit switches on reduced physics codes)
  - Gotta get designers to use them

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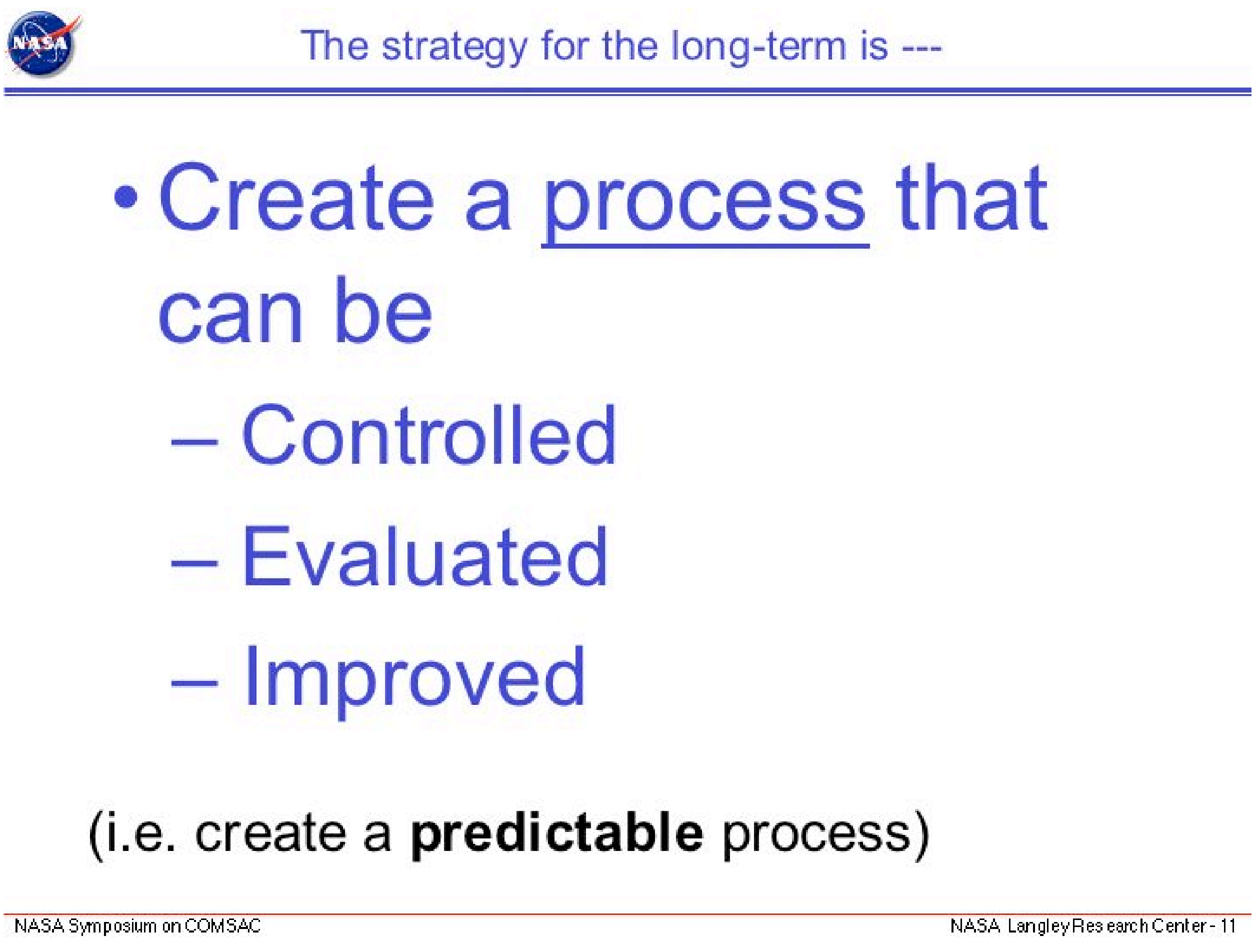
We recommend the following reference for further reading on process quality assurance:

M. C. Paulk, et al, “Capability Maturity Model for Software, Version 1.1”, Technical Report CMU/SEI-93-TR-024 (also ESC-TR-93-177), Software Engineering Institute, Carnegie Mellon University, February 1993 (download from SEI website).

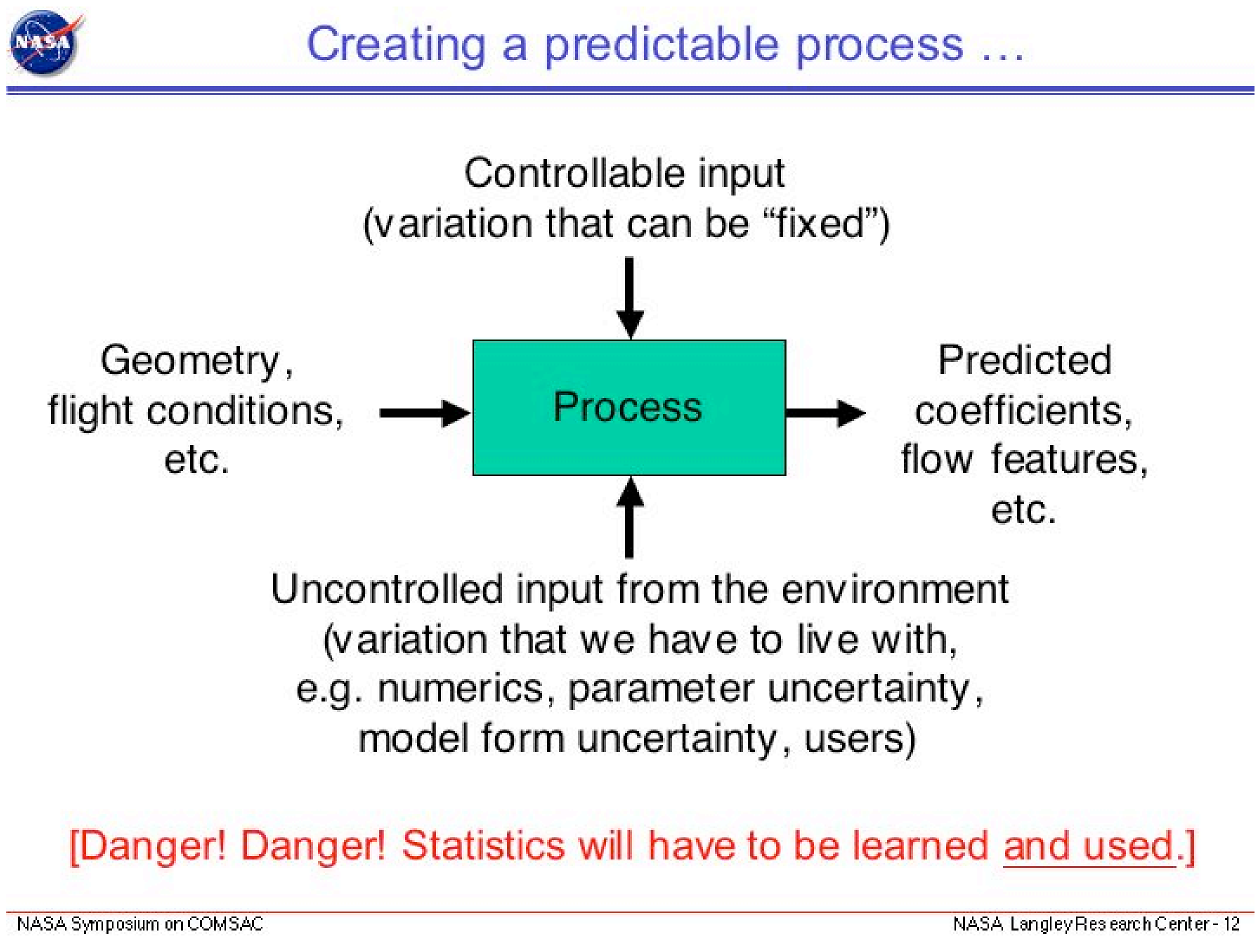
The above referenced document shows how to create and manage such a process. Paulk, et al have applied the approach to the software development process, but it applies just as well to any process, including uncertainty prediction/quantification.



We would like to note that often the very act of measuring the outcome of a process (Evaluation) will lead to improvement in the process result. This was evident in the improvement of the Second Drag Prediction Workshop results over those of the First. We have also seen this in our development of statistical control of wind tunnel measurement processes.

If we think of prediction as a manufacturing process, then we have the situation described schematically above. We would never expect every widget coming off the line to have identical dimensions and, similarly, we should not expect every prediction to have no variation across, codes, grid types, users, turbulence models, etc.

We do want to emphasize that to realize the full benefit of thinking this way and making it happen, it will be necessary to be fairly proficient at some basic statistical methods. The methods of greatest interest are the same ones used extensively in metrology and experimentation, particularly statistical quality/process control. Fortunately, these methods are not complicated. They do, however, require the user to get into a "statistical frame of mind" in order to use them effectively and correctly.



In this presentation, we talk a lot about processes because the notion is fundamental to quality assurance, especially quantitative quality assurance.

The best way that we know of to enable determination of quality is to think of computation as a process for manufacturing numbers. One of the biggest advantages of thinking this way is that we can borrow most of the methods and strategies of the manufacturing quality assurance community that have been developed over the last 80 years. In addition, we can borrow the extensions of those ideas to precision experimental work that have been developed at the National Bureau of Standards over the last 40 years.

Critical levels of attainment for a predictable process

- A defined set of steps
- Stable and replicable
- Measurable
- Improvable

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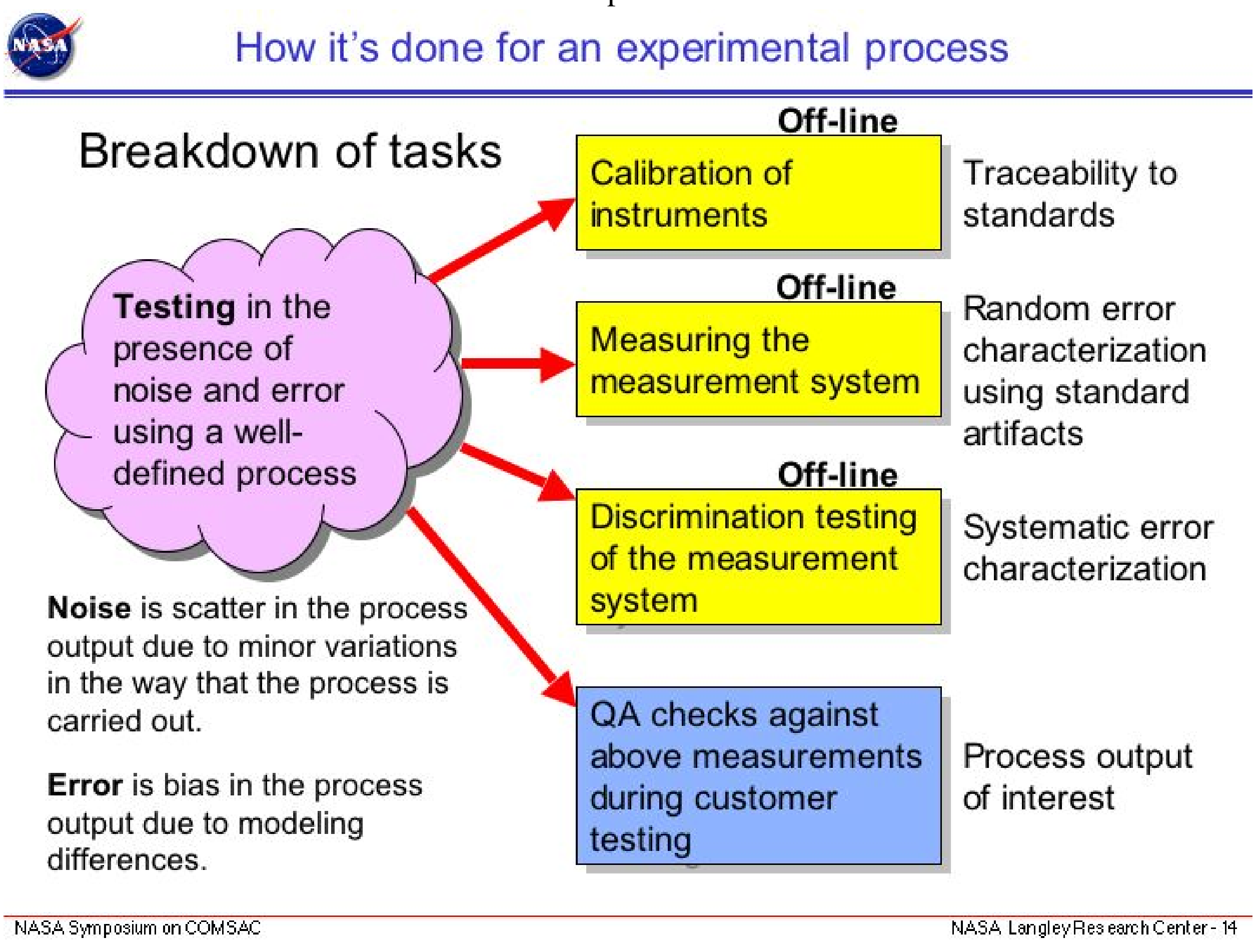
The quality assurance levels listed in the slide have been implicit in the quality literature but they were first promoted heavily by the Software Engineering Institute. (see reference on slide 11). These aspects are crucial for the credible **prediction** of computational uncertainty. The DoD actually has a process for certifying the quality assurance level attained on a sustained basis by a contractor's software development process, ranging from Level 1 (no process) to Level 5 (all of the above attributes are included).

This breakdown of tasks was established by the National Bureau of Standard over 40 years ago for precision measurement in standards and calibration labs. It makes a seemingly impossible task not only tractable but controllable and credible.

The first task, Calibration of Instruments, is done offline and provides a common reference state for all facilities which are traceable to national standards.

The second task involves periodic offline testing of the measurement system using standard artifacts which are called check standards. This task is done solely for the purposes of tracking any possible drift in the mean or dispersion of the measurement output of the system. It also allows the credible characterization of that dispersion.



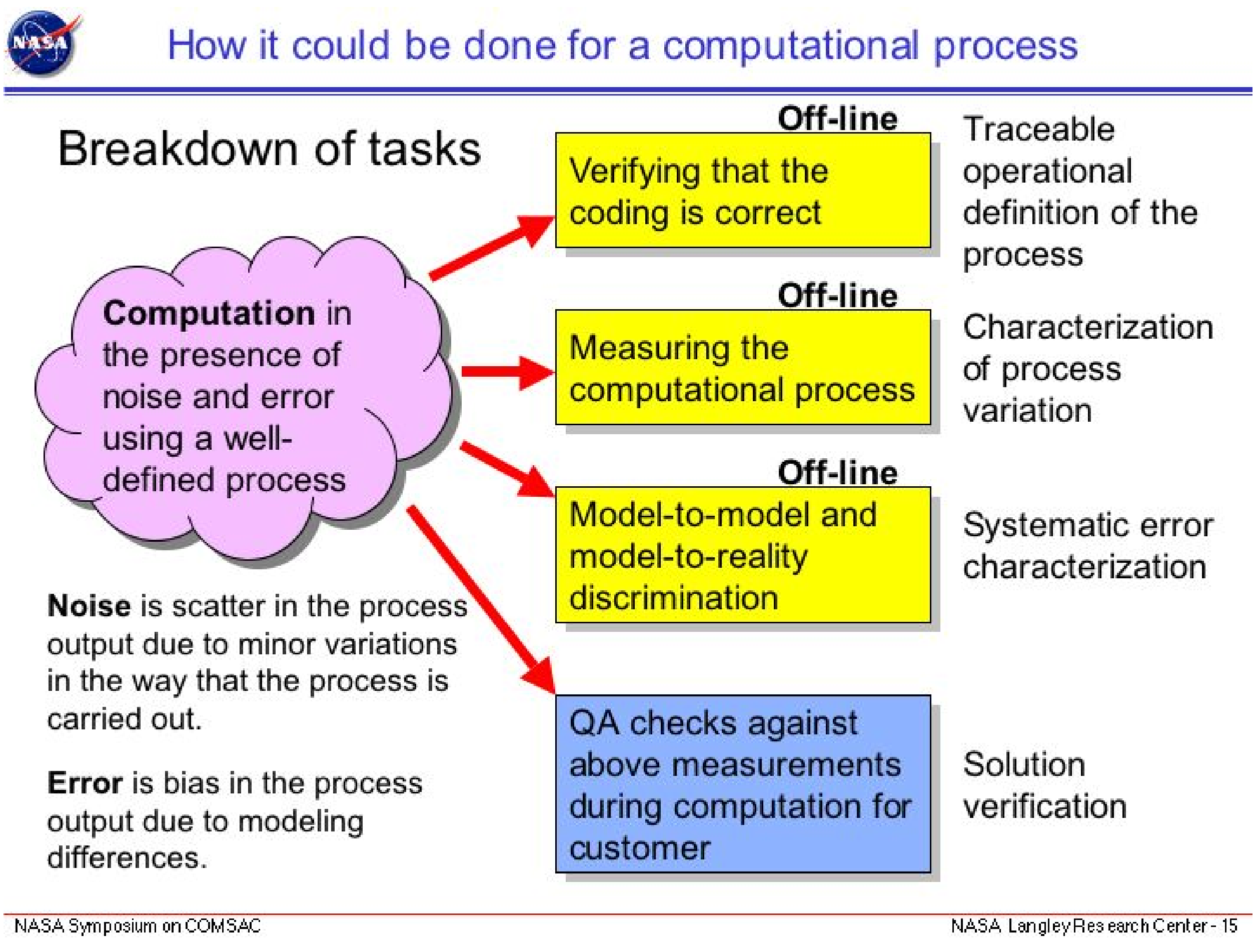
The third task involves the off-line determination of systematic errors in the measurement system. For a wind tunnel, some examples would be imperfect knowledge of the test section calibration coefficient and imperfect correction of wall effects.

The fourth task involves those quality checks to be conducted during a test. Those checks are conducted by comparing data taken during the test for that purpose against historical data. There are many such checks that need to be done in a wind tunnel test.

The first task again provides referenceability by being able to prove that the code is doing what it is purported to do. This task is usually called “Code Verification” (Roache)

The second task requires that the output variation of the computational process be controlled and evaluated. This can be effected through best practices and comparing the results of multiple codes, grid types, turbulence models, users, etc. There is a belief that attempts at grid convergence will be helpful here with part of this variation but preliminary results are not encouraging. This task is part of what is usually called “Solution Verification” (Roache).

The third task involves parameter and model form uncertainty. There are a variety of ways to propagate parameter uncertainty into the code output and we are encouraged that these methods not only work but



can be reasonably implemented. Model form uncertainty is another story and much work needs to be done here. The most promising notion that we’ve seen is the idea from statistics of “severe testing” in which one attempts to find both the portions of the envelope where the predictions are reliable and the accuracy can be evaluated and the boundaries of those portions where the predictions become less reliable and accuracy becomes more difficult to predict. This task is usually called “Validation” (Roache).

The fourth task involves checks to be made when a prediction is being made for a customer. Here it will be necessary (1) to assure that the best practice system is being followed so that predictions of process uncertainty have credibility and (2) to estimate the locations of the envelope boundaries where the credibility of the predicted systematic uncertainty becomes more problematical. This task is the on-line part of Solution Verification.

See http://aaac.larc.nasa.gov/tsab/cfdlarc/aiaa-dpw/.

Recommended actions for COMSAC **near-term**

- **Establish a working group like the AIAA Drag Prediction Workshop (DPW)**
  - Steer activities that can be started right now
  - Select a **small** number of COMSAC focus problems
  - Use those problems
    - » to demonstrate the prediction uncertainty strategies we've proposed
    - » to find out just how tough this problem really is
- **Some useful things to do right now for estimating uncertainty**
  - Run multiple codes, different grid types, multiple turbulence models, etc.
  - Stick to realistic S&C problems, i.e. work data sets that fully capture the physics of the problem of interest.

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Recommended actions for COMSAC **far-term**

- **Some key things to do right now to develop a powerful and reliable uncertainty quantification (UQ) process**
  - Help us establish a reasonable UQ process.
    - » Help us develop best practices and find ways to control and evaluate them.
    - » Help develop and implement tools for propagating parameter uncertainty and IC/BC uncertainty into the coefficients of interest.
    - » Help develop experiments to determine our ability to predict uncertainty and to predict the domain boundaries where the physics changes (and, therefore, probably the uncertainty).

We do not want, with the emphasis of this slide, to inadvertently give the impression that only on-line work counts. To the contrary, Slide 15 shows that we consider the off-line work described therein to be essential for a tractable and accurate process. By “local”, we simply mean local in the physical inference space (right physics).